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RESONANT PHOTOEMISSION STUDY OF $Sn_{0.96}Gd_{0.04}Te$

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$Sn_{0.96}Gd_{0.04}Te$ has been studied by means of the resonant photoemission spectroscopy in the constant final states, constant initial states and energy distribution curves modes. In the constant final states spectrum of the well-known giant resonance at the $4d$–$4f$ threshold around 150 eV we were able to resolve a peak of the multiplet structure that has not previously been found. Spectra were also taken at the $4p$–$5d$ threshold around 280 eV revealing a double structure with antiresonating behaviour.

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1. Introduction

It has been found very recently by Hall effect and magnetic susceptibility measurements that semimagnetic $Sn_{1-x}Gd_xTe$ with $x < 0.05$ shows completely new effects [1]. For instance, enhanced Gd–Gd exchange interaction and hole mobility, an order of magnitude higher for samples with $x < 0.05$ than for $x > 0.05$, were observed. A model was proposed with the $5d^1$ states hybridized to the heavy hole Σ-band and the light hole L-band. A first experimental hint for the location of the Gd $5d$ electrons was found by photoemission difference spectra of the ternary compound $Sn_{0.96}Gd_{0.04}Te$ and the binary one SnTe [2]. The latter result could be reproduced by our measurements.

To gain further insight into the electronic structure, especially the energy position of the unfilled $5d$ states and into the charge state of the Gd ion, we performed photoemission and resonant photoemission measurements at $Sn_{0.96}Gd_{0.04}Te$ and SnTe for comparison in the range of the $4p$–$5d$ threshold.

2. Experimental

The crystals were grown by the Bridgman method at the Polish Academy of Sciences and were cleaved by an anvil knife technique in an ultrahigh vacuum preparation system. Photoemission measurements in the energy distribution curves (EDC), constant final states (CFS) and constant initial states (CIS) modes were taken at the BW3 beam line of the storage ring DORIS at HASYLAB in Hamburg, Germany. Spectra were taken with a hemispherical analyzer. The overall energy resolution was chosen between 30 and 350 meV.

3. Results and discussion

For the description of the measured resonances the Fano formalism [3, 4] is used. For the emission of an electron two processes must be taken into account. Firstly, there is the direct process of photoemission into a continuum state, i.e

$$4d^{10}4f^7 + h\nu \rightarrow 4d^{10}4f^6 + e^-.$$

The other one is the autoionization via an excited discrete state

$$4d^{10}4f^7 + h\nu \rightarrow [4d^9 4f^8]^* \rightarrow 4d^{10}4f^6 + e^-.$$

Both processes lead to the same final state and can interfere with one another. In the case of the interference of one discrete state with one continuum the intensity of the emission is given by the Fano profile as follows:

$$N(E) = I_0 \frac{(\epsilon + q)^2}{\epsilon^2 + 1} \qquad (1)$$

with amplitude I_0, asymmetry parameter q and reduced energy $\epsilon = -2(E_{\mathrm{R}} - E)/\Gamma$, where E is the photon energy, E_{R} the location of the resonance and Γ the FWHM. For a least squares fitting procedure I_0, E_{R}, Γ and q are taken as parameters. The fits of the spectra were performed under the assumption of a linear background which was also determined by the fitting procedure.

The maximum of the Fano type giant resonance of Gd ($4d$–$4f$) was found at $h\nu = 149.3$ eV photon energy locating the $4f$ derived states 9.3 eV below the Fermi level. Compared to Ref. [2] a further peak in the multiplet structure of the $4d$–$4f$ resonance at $h\nu = 143.11$ could be resolved. On the whole, the CFS spectrum (Fig. 1) taken at an energy resolution of 30 meV looks like the yield spectrum of Gd metal [5]. The giant resonance is due to excited septet configurations whereas the two small structures at its onset are attributed to excited quintet configurations which can be reached by spin flip in the decay process. Comparing the CFS spectrum with that taken from Gd metal [5] which is assumed to be in a triply ionized state [6] it can be concluded that Gd is in the ionization state 3^+ in $Sn_{0.96}Gd_{0.04}Te$, too.

The three distinct structures of Fig. 1 can be fitted by the sum of three Fano profiles according to Eq. (1). The asymmetry parameters of the peaks are quite different. If q is small there is an interaction between the discrete and the continuum states [4], i.e. $q_3 = 3.2$ for the giant resonance. If $q = \infty$, Eq. (1) is equal to a Lorentzian. In the case of the quintet structures the asymmetry parameters are $q_1 = 29$ and $q_2 = 25$. As a result one gets quite symmetric peaks. So the interaction with the direct process is small.

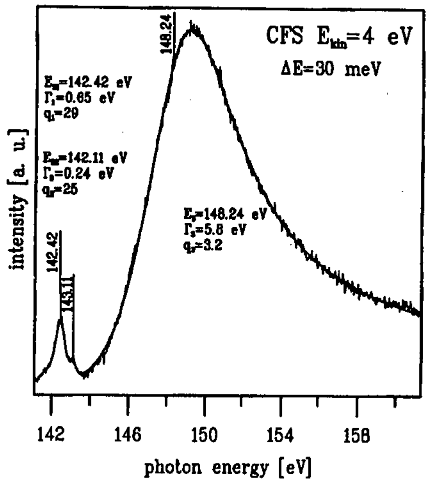

Fig. 1. Giant resonance at the Gd $4d$–$4f$ threshold.

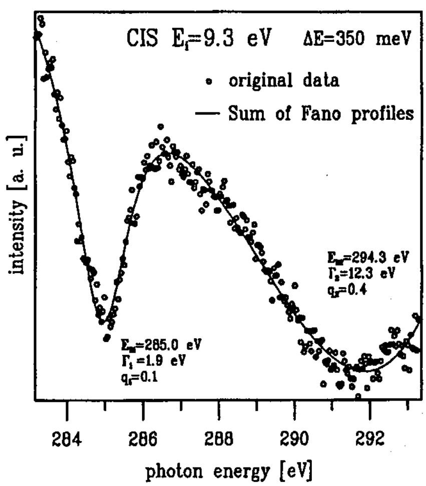

Fig. 2. CIS spectrum at the Gd $4p$–$5d$ threshold.

CIS and CFS spectra in the energy range of the transition from the Gd $4p_{1/2}$ to the unoccupied Gd $5d$ states reveal an antiresonating Fano type behaviour with two minima separated by 7 eV. Figure 2 shows a CIS spectrum in the energy range from 283 eV to 293 eV. In this case, the spectrum can be fitted by the sum of two Fano profiles according to Eq. (1) with asymmetry parameters $q_1 = 0.11$ and $q_2 = 0.4$ and spectral widths $\Gamma_1 = 1.9$ eV and $\Gamma_2 = 12.3$ eV. The fit is also shown in Fig. 2. Because of its comparatively small width the first minimum at 285 eV can be due to excitonic states whereas the second broad minimum around 292 eV can be attributed to conduction band states. As initial state for the CIS spectrum the $4f$ derived state at 9.3 eV was chosen. Obviously the Gd $4f$ state takes part in the resonance, i.e.

$$4p^6 4f^7 5d^1 \rightarrow [4p^5 4f^7 5d^2]^* \rightarrow 4p^6 4f^6 5d^1.$$

The resonance energy corresponds approximately to the binding energy of the Gd $4p_{1/2}$ core level. In Gd metal the Gd $4p_{1/2}$ level is found at 289 eV and the Gd $4p_{3/2}$ level at 268 eV binding energy. From energy considerations, we take this as an indication that the unfilled Gd $5d$ states are close to the conduction band minimum. In order to rule out artefacts, CIS spectra were taken from SnTe in the same energy range. In fact, they do not show any structure.

For the existence of the Gd $4p_{3/2}$ resonance around 268 eV we found only weak indications. We attribute this to the interaction of the spin–orbit with the exchange Hamiltonian as described in Ref. [7] leading to an intensity inversion of the $p_{1/2}$ and $p_{3/2}$ derived peaks.

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